

Derivatives of Feynman-Kac semigroups

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Abstract

We prove Bismut-type formulae for the first and second derivatives of a Feynman-Kac semigroup on a complete Riemannian manifold. We derive local estimates and give bounds on the logarithmic derivatives of the integral kernel. Stationary solutions are also considered. The arguments are based on local martingales, although the assumptions are purely geometric.

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1 Introduction

Suppose M is a complete Riemannian manifold of dimension n with Levi-Civita connection ∇ . Denote by Δ the Laplace-Beltrami operator, suppose Z is a smooth vector field and set $L := \frac{1}{2}\Delta + Z$. Any elliptic diffusion operator on a smooth manifold induces, via its principle symbol, a Riemannian metric with respect to which it takes this form. Denote by x_t a diffusion on M starting at $x_0 \in M$ with generator L and explosion time $\zeta(x_0)$. The explosion time is the random time at which the process leaves all compact subsets of M . Suppose $V : [0, \infty) \times M \rightarrow \mathbb{R}$ is a smooth function which is bounded below and denote by $P_t^V f$ the associated Feynman-Kac semigroup acting on bounded measurable functions f . For $T > 0$ fixed, $P_t^V f$ is smooth and bounded on $(0, T] \times M$, satisfies the parabolic equation

$$\partial_t \phi_t = (L - V_t) \phi_t \quad (1)$$

on $(0, T] \times M$ with $\phi_0 = f$ and for

$$\mathbb{V}_t := e^{-\int_0^t V_{T-s}(x_s) ds} \quad (2)$$

is represented probabilistically by the Feynman-Kac formula

$$P_T^V f(x_0) = \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \right]. \quad (3)$$

In the self-adjoint case, equation (1) corresponds, via Wick rotation, to the Schrödinger equation for a single non-relativistic particle moving in an electric field in curved space. In this sense, the derivative $dP_T^V f$ corresponds to the momentum of the particle and $LP_T^V f$ the kinetic energy. In this article we prove probabilistic formulae and estimates for $dP_T^V f$, $LP_T^V f$ and also for the Hessian $\nabla dP_T^V f$. These are the main results; they are summarized below.

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Our formula for $dP_T^V f$ is given by Theorem 2.2. For $v \in T_{x_0} M$ it states

$$(dP_T^V f)(v) = -\mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle W_s(\dot{k}_s v), //_s dB_s \rangle + dV_{T-s}(W_s(k_s v)) ds \right]$$

where $//_t$ and W_t are the usual parallel and damped parallel transports, respectively, and B_t the martingale part of the antidevelopment of x_t to $T_{x_0} M$. The process k_t is chosen so that it vanishes once x_t exits a regular domain (an open connected subset with compact closure and smooth boundary). In particular, no assumptions are required on the tensor Ric_Z . For the case in which Ric_Z is bounded below with $k_t = (T - t)/T$, our formula for $dP_t^V f$ reduces to that of [5, Theorem 5.2]. Formulae in [5] are derived from the assumption that one can differentiate under the expectation, and thus require global assumptions. Our approach, on the other hand, follows that of [17] and [1] in using local martingales to obtain local formula for which no assumptions are needed. For the case in which V is zero, our formula for $dP_t^V f$ reduces to that of [17].

Our formula for $LP_T^V f$ is given by Theorem 2.5. It states

$$\begin{aligned} & L(P_T^V f)(x_0) \\ = & \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle \dot{k}_s Z, //_s dB_s \rangle \right] \\ & + \frac{1}{2} \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \left(\int_0^T \langle W_s \dot{l}_s, //_s dB_s \rangle + dV_{T-s}(W_s l_s) ds \right) \int_0^T \dot{k}_s W_s^{-1} //_s dB_s \right] \end{aligned}$$

where the processes k and l are assumed to vanish outside of a regular domain. For the case $Z = 0$ and $V = 0$, a formula for ΔP_T acting on differential forms was given in [6]. Our formula therefore extends that result for the case of functions.

Our formula for $\nabla dP_T^V f$ is given by Theorem 2.7. For $v, w \in T_{x_0} M$ it states

$$\begin{aligned} & (\nabla dP_T^V f)(v, w) \\ = & -\mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle W'_s(\dot{k}_s v, w), //_s dB_s \rangle \right] \\ & - \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T ((\nabla dV_{T-s})(W_s(k_s v), W_s(w)) + (dV_{T-s})(W'_s(k_s v, w))) ds \right] \\ & + \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \left(\int_0^T \langle W_s(\dot{l}_s w), //_s dB_s \rangle + dV_{T-s}(W_s(l_s w)) ds \right) \right. \\ & \quad \left. \cdot \left(\int_0^T \langle W_s(\dot{k}_s v), //_s dB_s \rangle + dV_{T-s}(W_s(k_s v)) ds \right) \right] \end{aligned}$$

where W'_t solves a covariant Itô equation determined by the curvature tensor and its derivatives. This result extends [1, Theorem 2.1] which concerned the case $Z = 0$ and $V = 0$. Moreover our proof is more direct than the one given there in that it does not rely on the formulation of a stochastic differential equation. It instead uses a commutation relation based on the differential Bianchi identity.

The formulae mentioned above are derived in Section 2. Solutions to the time independent equation

$$(L - V)\phi = -E\phi$$

with $E \in \mathbb{R}$ are subject to a similar analysis, as outlined in Section 3. In Section 4 we use the formulae of Section 2 to derive local and global estimates. We do by choosing the processes k and l appropriately, as in [17] and [1], and applying the Cauchy-Schwarz inequality. The local estimates are given by Theorems 4.1, 4.3 and 4.5; the global estimates as corollaries. The global estimates imply the boundedness of $dP_t^V f$, $LP_t^V f$ and $\nabla dP_t^V f$ on $[\epsilon, T] \times M$. These bounds lead to the non-local formulae of Section 5, in which the processes k and l are chosen deterministically. For the case in which Z is gradient, global estimates on the logarithmic derivatives of the integral kernel can then be derived, using Jensen's inequality. These are given in Section 6. For the special case $V = 0$, local estimates for the gradient and Hessian can be found in [2] and [12], respectively. For the general case, our estimates extend the gradient and Hessian estimates of [8] and [16].

One application of our results is that they can be used to obtain formulae and estimates for the derivatives of the transition density $p_t^Z(x, y)$ of the diffusion with generator L in the *forward* variable y . This is because, according to the Fokker-Planck equation, one has the relation

$$p_t^Z(x, y) = p_t^{-Z, -\operatorname{div} Z}(y, x)$$

where $p_t^{-Z, -\operatorname{div} Z}(y, x)$ denotes the minimal integral kernel for the semigroup generated by the operator $L^* = \frac{1}{2}\Delta - Z - \operatorname{div} Z$. In particular, Bismut-type formulae for the derivatives in y of the right-hand side are given simply by conditioning in the formulae stated above (having replaced Z with $-Z$ and V with $-\operatorname{div} Z$). Further analysis of this problem, including a Bismut-type formula for the forward variable expressed in terms of the original diffusion, as opposed to its dual, will be considered in a subsequent article.

2 Local Formulae

For the remainder of this article, we fix $T > 0$ and set $f_t := P_{T-t}^V f(x_0)$.

2.1 Gradient

Denote by $\operatorname{Ric}_Z^\sharp := \operatorname{Ric}^\sharp - 2\nabla Z$ the Bakry-Emery tensor (see [3]). Then the damped parallel transport $W_t : T_{x_0}M \rightarrow T_{x_t}M$ is the solution, along the paths of x_t , to the covariant ordinary differential equation

$$DW_t = -\frac{1}{2}\operatorname{Ric}_Z^\sharp W_t$$

with $W_0 = \operatorname{id}_{T_{x_0}M}$. Suppose D is a regular domain in M with $x_0 \in D$ and denote by τ the first exit time of x_t from D .

Lemma 2.1. *Suppose $v \in T_{x_0}M$ and that k is a bounded adapted process with paths in the Cameron-Martin space $L^{1,2}([0, T]; \operatorname{Aut}(T_{x_0}M))$ such that $k_t = 0$ for $t \geq T - \epsilon$. Then*

$$\mathbb{V}_t df_t(W_t(k_t v)) - \mathbb{V}_t f_t(x_t) \int_0^t \langle W_s(\dot{k}_s v), / /_s dB_s \rangle - \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s(k_s v)) ds \quad (4)$$

is a local martingale on $[0, \tau \wedge T)$.

Proof. Setting $N_t(v) := df_t(W_t(v))$ we see by Itô's formula and the relations

$$\begin{aligned} d\Delta f &= \text{tr } \nabla^2 df - df(\text{Ric}^\#) \\ dZf &= \nabla_Z df + df(\nabla Z) \\ dV_t f &= f dV_t + V_t df \end{aligned}$$

(the first one is the Weitzenböck formula) that

$$\begin{aligned} dN_t(v) &\stackrel{m}{=} df_t(DW_t(v))dt + (\partial_t df_t)(W_t(v))dt + \left(\frac{1}{2} \text{tr } \nabla^2 + \nabla_Z\right)(df_t)(W_t(v))dt \\ &= V_{T-t}N_t(v)dt + f_t(x_t)dV_{T-t}(W_t(v))dt \end{aligned}$$

where $\stackrel{m}{=}$ denotes equality modulo the differential of a local martingale. Recalling the definition of V_t given by equation (2), it follows that

$$d(V_t N_t(k_t v)) \stackrel{m}{=} V_t N_t(\dot{k}_t v)dt + V_t f_t(x_t)dV_{T-t}(W_t(k_t v))dt$$

so that

$$V_t N_t(k_t v) - \int_0^t V_s df_s(W_s(\dot{k}_s v))ds - \int_0^t V_s f_s(x_s)dV(W_s(k_s v))ds$$

is a local martingale. By the formula

$$V_t f_t(x_t) = f_0(x_0) + \int_0^t V_s df_s(//_s dB_s)$$

and integration by parts we see that

$$\int_0^t V_s df_s(W_s(\dot{k}_s v))ds - V_t f_t(x_t) \int_0^t \langle W_s(\dot{k}_s v), //_s dB_s \rangle$$

is also a local martingale and so the lemma is proved. \square

Theorem 2.2. Suppose $x_0 \in D$ with $v \in T_{x_0}M$, $f \in \mathcal{B}_b$, V bounded below and $T > 0$. Suppose k is a bounded adapted process with paths in the Cameron-Martin space $L^{1,2}([0, T]; \text{Aut}(T_{x_0}M))$ such that $k_0 = 1$, $k_t = 0$ for $t \geq \tau \wedge T$ and $\int_0^{\tau \wedge T} |\dot{k}_s|^2 ds \in L^1$. Then

$$(dP_T^V f)(v) = -\mathbb{E} \left[V_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle W_s(\dot{k}_s v), //_s dB_s \rangle + dV_{T-s}(W_s(k_s v))ds \right]. \quad (5)$$

Proof. As in the proof of [17, Theorem 2.3], the process k_t can be modified to k_t^ϵ so that $k_t^\epsilon = k_t$ for $t \leq \tau \wedge (T - 2\epsilon)$ and $k_t^\epsilon = 0$ for $t \geq \tau \wedge (T - \epsilon)$, cutting off appropriately in between. Since $(df_t)_x$ is smooth and therefore bounded for $(t, x) \in [0, T - \epsilon] \times D$, it follows from Lemma 2.1 and the strong Markov property that formula (5) holds with k_t^ϵ in place of k_t . The result follows by taking $\epsilon \downarrow 0$. \square

2.2 Generator

Now suppose D_1 and D_2 are regular domains with $x_0 \in D_1$ and $\overline{D_1} \subset D_2$. Denote by σ and τ the first exit times of x_t from D_1 and D_2 , respectively.

Lemma 2.3. Suppose $x_0 \in D_1$ and $0 < S < T$ and that k, l are bounded adapted processes with paths in the Cameron-Martin space $L^{1,2}([0, T]; \mathbb{R})$ such that $k_s = 0$ for

$s \geq \sigma \wedge S$, $l_s = 1$ for $s \leq \sigma \wedge S$ and $l_s = 0$ for $s \geq \tau \wedge (T - \epsilon)$. Then

$$\begin{aligned} & \mathbb{V}_t(Lf_t)(x_t)k_t - \frac{1}{2}\mathbb{V}_tdf_t\left(W_t l_t \int_0^t \dot{k}_s W_s^{-1} //_s dB_s\right) \\ & + \frac{1}{2}\mathbb{V}_t f_t(x_t) \int_0^t \langle W_s \dot{l}_s, //_s dB_s \rangle \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \\ & \frac{1}{2} \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s l_s) ds \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \\ & + \mathbb{V}_t f_t(x_t) \int_0^t \langle \dot{k}_s Z - k_s \nabla V_{T-s}, //_s dB_s \rangle \\ & - \int_0^t \mathbb{V}_s f_s k_s LV_{T-s} ds \end{aligned}$$

is a local martingale on $[0, \tau \wedge T)$.

Proof. Defining

$$n_t := (Lf_t)(x_t)$$

we have, by Itô's formula, that

$$\begin{aligned} dn_t &= d(Lf_t)_{x_t} //_t dB_t + \partial_t(Lf_t)(x_t)dt + L(Lf_t)(x_t)dt \\ &= d(Lf_t)_{x_t} //_t dB_t + L(V_{T-t}f_t)dt \\ &= d(Lf_t)_{x_t} //_t dB_t + (LV_{T-t})f_t dt + V_{T-t}n_t dt + \langle df_t, dV_{T-t} \rangle dt. \end{aligned}$$

It follows that

$$d(\mathbb{V}_t n_t k_t) \stackrel{m}{=} \mathbb{V}_t n_t \dot{k}_t + k_t \mathbb{V}_t (f_t LV_{T-t} + \langle df_t, dV_{T-t} \rangle) dt$$

and so

$$\mathbb{V}_t(Lf_t)(x_t)k_t - \int_0^t \mathbb{V}_s(Lf_s)(x_s) \dot{k}_s ds - \int_0^t \mathbb{V}_s k_s (f_s LV_{T-s} + \langle df_s, dV_{T-s} \rangle) ds$$

is a local martingale, with

$$-(Lf_t)(x_t) \dot{k}_t dt = \left(\frac{1}{2} d^* d - Z \right) f_t(x_t) \dot{k}_t dt = \left(\frac{1}{2} d^*(df_t) - (df_t)(Z) \right) \dot{k}_t dt.$$

By the Weitzenbock formula

$$d(\mathbb{V}_t(df_t)(W_t)) = (\nabla_{//_t dB_t} df_t)(W_t) - V_{T-t}(df_t)(W_t)dt + f_t(x_t) dV_{T-t}(W_t)dt$$

from which it follows that

$$d(\mathbb{V}_t(df_t)(W_t)) = \mathbb{V}_t(\nabla_{//_t dB_t} df_t)(W_t) + \mathbb{V}_t f_t(x_t) dV_{T-t}(W_t)dt.$$

Consequently, for an orthonormal basis $\{e_i\}_{i=1}^n$ of $T_{x_0}M$, by integration by parts we have

$$\begin{aligned} \mathbb{V}_t d^*(df_t) \dot{k}_t dt &= - \sum_{i=1}^n \mathbb{V}_t(\nabla_{//_t e_i} df_t)(//_t e_i) \dot{k}_t dt \\ &\stackrel{m}{=} - \mathbb{V}_t(\nabla_{//_t dB_t} df_t)(W_t) \dot{k}_t W_t^{-1} //_t dB_t \\ &= - d(\mathbb{V}_t df_t(W_t) \int_0^t \dot{k}_s W_s^{-1} //_s dB_s) \\ &\quad + d\left(\int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s) ds \int_0^t \dot{k}_s W_s^{-1} //_s dB_s\right). \end{aligned}$$

Furthermore

$$\int_0^t \mathbb{V}_s df_s(Z) \dot{k}_s ds - \mathbb{V}_t f_t(x_t) \int_0^t \langle \dot{k}_s Z, //_s dB_s \rangle$$

is a local martingale and therefore

$$\begin{aligned} & \int_0^t \mathbb{V}_s(Lf_s)(x_s) \dot{k}_s ds \\ & - \frac{1}{2} \mathbb{V}_t df_t(W_t) \int_0^t \dot{k}_s W_s^{-1} //_s dB_s + \frac{1}{2} \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s) ds \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \\ & + \mathbb{V}_t f_t(x_t) \int_0^t \langle \dot{k}_s Z, //_s dB_s \rangle \end{aligned}$$

is also a local martingale. By the assumptions on k and l it follows from Lemma 2.1 that

$$\begin{aligned} O_t^1 &= \mathbb{V}_t df_t(W_t((l_t - 1))) - \mathbb{V}_t f_t(x_t) \int_0^t \langle W_s(\dot{l}_s), //_s dB_s \rangle \\ & - \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s((l_s - 1))) ds, \\ O_t^2 &= \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \end{aligned}$$

are two local martingales. So the product $O_t^1 O_t^2$ is also a local martingale, since $O^1 = 0$ on $[0, \sigma \wedge S]$ with O^2 constant on $[\sigma \wedge S, \tau \wedge (T - \epsilon))$. Consequently

$$\begin{aligned} & - \mathbb{V}_t df_t \left(W_t \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \right) + \mathbb{V}_t df_t \left(W_t l_t \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \right) \\ & - \mathbb{V}_t f_t(x_t) \int_0^t \langle W_s \dot{l}_s, //_s dB_s \rangle \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \\ & - \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s((l_s - 1))) ds \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \end{aligned}$$

is a local martingale and therefore so is

$$\begin{aligned} & \mathbb{V}_t(Lf_t)(x_t) k_t - \frac{1}{2} \mathbb{V}_t df_t \left(W_t l_t \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \right) \\ & + \frac{1}{2} \mathbb{V}_t f_t(x_t) \int_0^t \langle W_s \dot{l}_s, //_s dB_s \rangle \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \\ & + \frac{1}{2} \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s l_s) ds \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \\ & + \mathbb{V}_t f_t(x_t) \int_0^t \langle \dot{k}_s Z, //_s dB_s \rangle \\ & - \int_0^t \mathbb{V}_s k_s (f_s LV_{T-s} + \langle df_s, dV_{T-s} \rangle) ds. \end{aligned}$$

Since

$$\int_0^t \mathbb{V}_s df_s(\nabla V_{T-s}) k_s ds - \mathbb{V}_t f_t(x_t) \int_0^t \langle k_s \nabla V_{T-s}, //_s dB_s \rangle$$

is a local martingale, the result follows. \square

Lemma 2.4. Suppose $x_0 \in D_1$, $f \in \mathcal{B}_b$, V bounded below and $0 < S < T$. Suppose k is a bounded adapted process with paths in the Cameron-Martin space $L^{1,2}([0, T]; \mathbb{R})$ such that $k_s = 0$ for $s \geq \sigma \wedge S$, $k_0 = 1$ and $\int_0^{\sigma \wedge S} |\dot{k}_s|^2 ds \in L^1$. Then

$$V_T(x_0)P_T^V f(x_0) = \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T (k_s \dot{V}_{T-s}(x_s) - \dot{k}_s V_{T-s}(x_s)) ds \right].$$

Proof. By Itô's formula, we have

$$d(\mathbb{V}_t V_{T-t} f_t k_t) \stackrel{m}{=} -k_t \mathbb{V}_t \dot{V}_{T-t} f_t + \dot{k}_t \mathbb{V}_t V_{T-t} f_t$$

which implies

$$\mathbb{V}_t V_{T-t} f_t k_t - \int_0^t (\dot{k}_s \mathbb{V}_s V_{T-s} f_s - k_s \mathbb{V}_s \dot{V}_{T-s} f_s) ds$$

is a local martingale on $[0, \tau \wedge T)$. The assumptions on f and V imply it is a martingale on $[0, \tau \wedge T]$, so result follows by taking expectations and applying the strong Markov property. \square

Theorem 2.5. Suppose $x_0 \in D_1$, $f \in \mathcal{B}_b$, V bounded below and $0 < S < T$. Suppose k, l are bounded adapted processes with paths in the Cameron-Martin space $L^{1,2}([0, T]; \mathbb{R})$ such that $k_s = 0$ for $s \geq \sigma \wedge S$, $k_0 = 1$, $l_s = 1$ for $s \leq \sigma \wedge S$, $l_s = 0$ for $s \geq \tau \wedge T$, $\int_0^{\sigma \wedge S} |\dot{k}_s|^2 ds \in L^1$ and $\int_{\sigma \wedge S}^{\tau \wedge T} |\dot{l}_s|^2 ds \in L^1$. Then

$$\begin{aligned} & L(P_T^V f)(x_0) \\ &= \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle \dot{k}_s Z, //_s dB_s \rangle \right] \\ &+ \frac{1}{2} \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \left(\int_0^T \langle W_s \dot{l}_s, //_s dB_s \rangle + dV_{T-s}(W_s l_s) ds \right) \int_0^T \dot{k}_s W_s^{-1} //_s dB_s \right]. \end{aligned}$$

Proof. Modifying the process l_t to l_t^ϵ as in the proof of Theorem 2.2, it follows from Lemma 2.3, the strong Markov property, the boundedness of $P_t^V f$ on $[0, T] \times \overline{D}_2$ and the boundedness of $dP_t^V f$ and $LP_t^V f$ on $[\epsilon, T] \times \overline{D}_2$ that the formula

$$\begin{aligned} & L(P_T^V f)(x_0) \\ &= \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \left(\int_0^T \langle \dot{k}_s Z, //_s dB_s \rangle - \int_0^T k_s (dV_{T-s} //_s dB_s) + LV_{T-s} ds \right) \right] \\ &+ \frac{1}{2} \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \left(\int_0^T \langle W_s \dot{l}_s, //_s dB_s \rangle + dV_{T-s}(W_s l_s) ds \right) \int_0^T \dot{k}_s W_s^{-1} //_s dB_s \right] \end{aligned}$$

holds with l_t^ϵ in place of l_t . The formula also holds as stated, in terms of l_t , by taking $\epsilon \downarrow 0$. Applying the Itô formula yields

$$\int_0^T k_s (dV_{T-s} //_s dB_s) + LV_{T-s} ds = -V_T(x_0) + \int_0^T (k_s \dot{V}_{T-s}(x_s) - \dot{k}_s V_{T-s}(x_s)) ds$$

and therefore

$$\begin{aligned}
& (L - V_T(x_0))(P_T^V f)(x_0) \\
= & \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \left(\int_0^T \langle \dot{k}_s Z, //_s dB_s \rangle - \int_0^T (k_s \dot{V}_{T-s}(x_s) - \dot{k}_s V_{T-s}(x_s)) ds \right) \right] \\
& + \frac{1}{2} \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \left(\int_0^T \langle W_s \dot{l}_s, //_s dB_s \rangle + dV_{T-s}(W_s l_s) ds \right) \int_0^T \dot{k}_s W_s^{-1} //_s dB_s \right].
\end{aligned}$$

The result follows from this by Lemma 2.4. \square

2.3 Hessian

For each $w \in T_{x_0} M$ define an operator-valued process $W'_t(\cdot, w) : T_{x_t} M \rightarrow T_{x_t} M$ by

$$\begin{aligned}
W'_s(\cdot, w) := & W_s \int_0^s W_r^{-1} R(//_r dB_r, W_r(\cdot)) W_r(w) \\
& - \frac{1}{2} W_s \int_0^s W_r^{-1} (\nabla \text{Ric}_Z^\# + d^* R)(W_r(\cdot), W_r(w)) dr.
\end{aligned}$$

The operator $d^* R$ is defined by $d^* R(v_1)v_2 := -\text{tr } \nabla \cdot R(\cdot, v_1)v_2$ and satisfies

$$\langle d^* R(v_1)v_2, v_3 \rangle = \langle (\nabla_{v_3} \text{Ric}^\#)(v_1), v_2 \rangle - \langle (\nabla_{v_2} \text{Ric}^\#)(v_3), v_1 \rangle$$

for all $v_1, v_2, v_3 \in T_x M$ and $x \in M$. The process $W'_t(\cdot, w)$ is the solution to the covariant Itô equation

$$\begin{aligned}
DW'_t(\cdot, w) = & R(//_t dB_t, W_t(\cdot)) W_t(w) \\
& - \frac{1}{2} \left(d^* R + \nabla \text{Ric}_Z^\# \right) (W_t(\cdot), W_t(w)) dt \\
& - \frac{1}{2} \text{Ric}_Z^\#(W'_t(\cdot, w)) dt
\end{aligned}$$

with $W'_0(\cdot, w) = 0$. As in the previous section, suppose D_1 and D_2 are regular domains with $x_0 \in D_1$ and $\overline{D_1} \subset D_2$. Denote by σ and τ the first exit times of x_t from D_1 and D_2 , respectively.

Lemma 2.6. *Suppose $v, w \in T_{x_0} M$, $0 < S < T$ and that k, l are bounded adapted processes with paths in the Cameron-Martin space $L^{1,2}([0, T]; \text{Aut}(T_{x_0} M))$ such that $k_s = 0$ for $s \geq \sigma \wedge S$, $l_s = 1$ for $s \leq \sigma \wedge T$ and $l_s = 0$ for $s \geq \tau \wedge (T - \epsilon)$. Then*

$$\begin{aligned}
& \mathbb{V}_t(\nabla df_t)(W_t(k_t v), W_t(w)) + \mathbb{V}_t(df_t)(W'_t(k_t v, w)) - \mathbb{V}_t f_t(x_t) \int_0^t \langle W'_s(\dot{k}_s v, w), //_s dB_s \rangle \\
& - \int_0^t \mathbb{V}_s f_s(x_s) ((\nabla dV_{T-s})(W_s(k_s v), W_s(w)) + (dV_{T-s})(W'_s(k_s v, w))) ds \\
& + \mathbb{V}_t f_t(x_t) \int_0^t \langle W_s(\dot{l}_s w), //_s dB_s \rangle \int_0^t \langle W_s(\dot{k}_s v), //_s dB_s \rangle \\
& - \mathbb{V}_t df_t(W_t(l_t w)) \int_0^t \langle W_s(\dot{k}_s v), //_s dB_s \rangle \\
& + \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s((l_s - 1)w)) ds \int_0^t \langle W_s(\dot{k}_s v), //_s dB_s \rangle \\
& + \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s(w)) \int_0^s \langle W_r(\dot{k}_r v), //_r dB_r \rangle ds
\end{aligned}$$

$$- 2 \int_0^t \mathbb{V}_s(df_s \odot dV_{T-s})(W_s(k_s v), W_s(w)) ds \quad (2)$$

is a local martingale on $[0, \tau \wedge T)$.

Proof. Setting

$$N'_t(v, w) := (\nabla df_t)(W_t(v), W_t(w)) + (df_t)(W'_t(v, w))$$

and

$$R_x^{\sharp, \sharp}(v_1, v_2) := R_x(\cdot, v_1, v_2, \cdot)^{\sharp} \in T_x M \otimes T_x M$$

we see by Itô's formula and the relations

$$\begin{aligned} d\Delta f &= \text{tr } \nabla^2 df - df(\text{Ric}^{\sharp}) \\ dZ f &= \nabla_Z df + df(\nabla Z) \\ dV f &= f dV + V df \\ \nabla d(\Delta f) &= \text{tr } \nabla^2(\nabla df) - 2(\nabla df)(\text{Ric}^{\sharp} \odot \text{id} - R^{\sharp, \sharp}) - df(d^* R + \nabla \text{Ric}^{\sharp}) \\ \nabla d(Z f) &= \nabla_Z(\nabla df) + 2(\nabla df)(\nabla Z \odot \text{id}) + df(\nabla \nabla Z) \\ \nabla d(V_t f) &= f \nabla dV_t + 2df \odot dV_t + V_t \nabla df \end{aligned}$$

(the fourth one is a consequence of the differential Bianchi identity; see [4, p. 219]) that

$$\begin{aligned} & dN'_t(v, w) \\ &= (\nabla_{//t dB_t} \nabla df_t)(W_t(v), W_t(w)) + (\nabla df_t) \left(\frac{D}{dt} W_t(v), W_t(w) \right) dt \\ &+ (\nabla df_t) \left(W_t(v), \frac{D}{dt} W_t(w) \right) dt \\ &+ \partial_t(\nabla df_t)(W_t(v), W_t(w)) dt + \left(\frac{1}{2} \text{tr } \nabla^2 + \nabla_Z \right) (\nabla df_t)(W_t(v), W_t(w)) dt \\ &+ (\nabla_{//t dB_t} df_t)(W'_t(v, w)) + (df_t)(DW'_t(v, w)) + \langle d(df_t), DW'_t(v, w) \rangle \\ &+ \partial_t(df_t)(W'_t(v, w)) dt + \left(\frac{1}{2} \text{tr } \nabla^2 + \nabla_Z \right) (df_t)(W'_t(v, w)) dt \\ &\stackrel{m}{=} f_t(x_t)(\nabla dV_{T-t})(W_t(v), W_t(w)) dt + f_t(x_t)(dV_{T-t})(W'_t(v, w)) dt \\ &+ 2(df_t \odot dV_{T-t})(W_t(v), W_t(w)) dt + V_{T-t} N'_t(v, w) dt \end{aligned}$$

for which we calculated

$$[d(df), DW'(v, w)]_t = (\nabla df_t)(R^{\sharp, \sharp}(W_t(v), W_t(w))) dt.$$

It follows that

$$\begin{aligned} d(\mathbb{V}_t N'_t(k_t v, w)) &\stackrel{m}{=} \mathbb{V}_t f_t(x_t)((\nabla dV_{T-t})(W_t(k_t v), W_t(w)) + (dV_{T-t})(W'_t(k_t v, w))) dt \\ &+ \mathbb{V}_t N_t(\dot{k}_t v, w) dt + 2\mathbb{V}_t(df_t \odot dV_{T-t})(W_t(k_t v), W_t(w)) dt \end{aligned}$$

so that

$$\begin{aligned} & \mathbb{V}_t N'_t(k_t v, w) - \int_0^t \mathbb{V}_s(\nabla df_s)(W_s(\dot{k}_s v), W_s(w)) ds - \int_0^t \mathbb{V}_s(df_s)(W'_s(\dot{k}_s v, w)) ds \\ & - 2 \int_0^t \mathbb{V}_s(df_s \odot dV_{T-s})(W_s(k_s v), W_s(w)) ds \\ & - \int_0^t \mathbb{V}_s f_s(x_s)((\nabla dV_{T-s})(W_s(k_s v), W_s(w)) + (dV_{T-s})(W'_s(k_s v, w))) ds \end{aligned}$$

is a local martingale. By the formula

$$\mathbb{V}_t f_t(x_t) = f_0(x_0) + \int_0^t \mathbb{V}_s df_s(//_s dB_s)$$

and integration by parts we see that

$$\int_0^t \mathbb{V}_s(df_s)(W'_s(\dot{k}_s v, w))ds - \mathbb{V}_t f_t(x_t) \int_0^t \langle W'_s(\dot{k}_s v, w), //_s dB_s \rangle$$

is a local martingale. Similarly, by the formula

$$\mathbb{V}_t df_t(W_t) = df_0 + \int_0^t \mathbb{V}_s(\nabla df_s)(//_s dB_s, W_s) + \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s) ds$$

and integration by parts we see that

$$\begin{aligned} & \int_0^t \mathbb{V}_s(\nabla df_s)(W_s(\dot{k}_s v), W_s(w))ds - \mathbb{V}_t df_t(W_t(w)) \int_0^t \langle W_s(\dot{k}_s v), //_s dB_s \rangle \\ & + \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s(w)) \int_0^s \langle W_r(\dot{k}_r v), //_r dB_r \rangle ds \end{aligned}$$

is yet another local martingale. Therefore

$$\begin{aligned} & \mathbb{V}_t(\nabla df_t)(W_t(k_t v), W_t(w)) + \mathbb{V}_t(df_t)(W'_t(k_t v, w)) \\ & - \int_0^t \mathbb{V}_s f_s(x_s)((\nabla dV_{T-s})(W_s(k_s v), W_s(w)) + (dV_{T-s})(k_s W'_s(v, w)))ds \\ & - \mathbb{V}_t f_t(x_t) \int_0^t \langle W'_s(\dot{k}_s v, w), //_s dB_s \rangle - 2 \int_0^t \mathbb{V}_s(df_s \odot dV_{T-s})(W_s(k_s v), W_s(w))ds \\ & + \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s(w)) \int_0^s \langle W_r(\dot{k}_r v), //_r dB_r \rangle ds \\ & - \mathbb{V}_t df_t(W_t(w)) \int_0^t \langle W_s(\dot{k}_s v), //_s dB_s \rangle \end{aligned}$$

is a local martingale. By Lemma 2.1 it follows that

$$\begin{aligned} O_t^1 &= \mathbb{V}_t df_t(W_t((l_t - 1)w)) - \mathbb{V}_t f_t(x_t) \int_0^t \langle W_s(\dot{l}_s w), //_s dB_s \rangle \\ & - \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s((l_s - 1)w))ds, \\ O_t^2 &= \int_0^t \langle W_s(\dot{k}_s v), //_s dB_s \rangle \end{aligned}$$

are two local martingales. So the product $O_t^1 O_t^2$ is also a local martingale, since $O^1 = 0$ on $[0, \sigma \wedge S]$ with O^2 constant on $[\sigma \wedge S, \tau \wedge (T - \epsilon))$. Applying this fact to the previous equation completes the proof. \square

Theorem 2.7. Suppose $x_0 \in D_1$ with $v, w \in T_{x_0} M$, $f \in \mathcal{B}_b$, V bounded below and $0 < S < T$. Assume k, l are bounded adapted processes with paths in the Cameron-Martin space $L^{1,2}([0, T]; \text{Aut}(T_{x_0} M))$ such that $k_s = 0$ for $s \geq \sigma \wedge S$, $k_0 = 1$, $l_s = 1$ for

$s \leq \sigma \wedge S$, $l_s = 0$ for $s \geq \tau \wedge T$, $\int_0^{\sigma \wedge S} |\dot{k}_s|^2 ds \in L^1$ and $\int_{\sigma \wedge S}^{\tau \wedge T} |\dot{l}_s|^2 ds \in L^1$. Then

$$\begin{aligned}
& (\nabla dP_T^V f)(v, w) \\
&= -\mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle W'_s(\dot{k}_s v, w), //_s dB_s \rangle \right] \\
&\quad - \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T ((\nabla dV_{T-s})(W_s(k_s v), W_s(w)) + (dV_{T-s})(W'_s(k_s v, w))) ds \right] \\
&\quad + \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \left(\int_0^T \langle W_s(\dot{l}_s w), //_s dB_s \rangle + dV_{T-s}(W_s(l_s w)) ds \right) \right. \\
&\quad \quad \left. \cdot \left(\int_0^T \langle W_s(\dot{k}_s v), //_s dB_s \rangle + dV_{T-s}(W_s(k_s v)) ds \right) \right].
\end{aligned}$$

Proof. Modifying the process l_t to l_t^ϵ as in the proof of Theorem 2.2, it follows from Lemma 2.6, the strong Markov property, the boundedness of $P_t^V f$ on $[0, T] \times \overline{D}_2$ and the boundedness of $dP_t^V f$ and $\nabla dP_t^V f$ on $[\epsilon, T] \times \overline{D}_2$ that the formula

$$\begin{aligned}
& (\nabla dP_T^V f)(v, w) \\
&= -\mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle W'_s(\dot{k}_s v, w), //_s dB_s \rangle \right] \\
&\quad + \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle W_s(\dot{l}_s w), //_s dB_s \rangle \int_0^T \langle W_s(\dot{k}_s v), //_s dB_s \rangle \right] \\
&\quad - \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T ((\nabla dV_{T-s})(W_s(k_s v), W_s(w)) + (dV_{T-s})(W'_s(k_s v, w))) ds \right] \\
&\quad + \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T dV_{T-s}(W_s(l_s w)) ds \int_0^T \langle W_s(\dot{k}_s v), //_s dB_s \rangle \right] \\
&\quad - \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \left(\int_0^s dV(W_r(w)) dr \right) \langle W_s(\dot{k}_s v), //_s dB_s \rangle \right] \\
&\quad - \mathbb{E} \left[\int_0^T \mathbb{V}_s df_s(W_s(k_s v)) dV_{T-s}(W_s(w)) ds \right] \\
&\quad - \mathbb{E} \left[\int_0^T \mathbb{V}_s df_s(W_s(w)) dV_{T-s}(W_s(k_s v)) ds \right]
\end{aligned}$$

holds with l_t^ϵ in place of l_t , and therefore in terms of l_t by taking $\epsilon \downarrow 0$. Paying close attention to the assumptions on l and k , it follows from this, by Theorem 2.2 and the strong Markov property, that

$$\begin{aligned}
& -\mathbb{E} \left[\int_0^T \mathbb{V}_s df_s(W_s(w)) dV_{T-s}(W_s(k_s v)) ds \right] \\
&= +\mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \int_r^T \langle W_s(\dot{l}_s w), //_s dB_s \rangle dV_{T-r}(W_r(k_r v)) dr \right] \\
&\quad - \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \left(\int_0^r dV_{T-u}(W_u(w)) du \right) dV_{T-r}(W_r(k_r v)) dr \right]
\end{aligned}$$

$$\begin{aligned}
& + \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T dV_{T-r}(W_r(k_r v)) dr \int_0^T dV_{T-s}(W_s(l_s w)) ds \right] \\
= & + \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle W_s(\dot{l}_s w), //_s dB_s \rangle \int_0^T dV_{T-r}(W_r(k_r v)) dr \right] \\
& - \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \left(\int_0^r dV_{T-u}(W_u(w)) du \right) dV_{T-r}(W_r(k_r v)) dr \right] \\
& + \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T dV_{T-r}(W_r(k_r v)) dr \int_0^T dV_{T-s}(W_s(l_s w)) ds \right]
\end{aligned}$$

from which it follows that

$$\begin{aligned}
& (\nabla dP_T^V f)(v, w) \\
= & - \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle W'_s(\dot{k}_s v, w), //_s dB_s \rangle \right] \\
& + \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle W_s(\dot{l}_s w), //_s dB_s \rangle \int_0^T \langle W_s(\dot{k}_s v), //_s dB_s \rangle \right] \\
& - \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T ((\nabla dV_{T-s})(W_s(k_s v), W_s(w)) + (dV_{T-s})(W'_s(k_s v, w))) ds \right] \\
& + \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T dV_{T-s}(W_s(l_s w)) ds \int_0^T \langle W_s(\dot{k}_s v), //_s dB_s \rangle \right] \\
& + \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle W_s \dot{l}_s w, //_s dB_s \rangle \int_0^T dV_{T-r}(W_r(k_r v)) dr \right] \\
& + \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T dV_{T-r}(W_r(k_r v)) dr \int_0^T dV_{T-s}(W_s(l_s w)) ds \right] \\
& - \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \left(\int_0^s dV_{T-r}(W_r(w)) dr \right) \langle W_s(\dot{k}_s v), //_s dB_s \rangle \right] \\
& - \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \left(\int_0^s dV_{T-r}(W_r(w)) dr \right) dV_{T-s}(W_s(k_s v)) ds \right] \\
& - \mathbb{E} \left[\int_0^T \mathbb{V}_s df_s(W_s(k_s v)) dV_{T-s}(W_s(w)) ds \right].
\end{aligned}$$

Finally, by the stochastic Fubini theorem [19, Theorem 2.2] we have

$$\begin{aligned}
& \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \int_0^s dV_{T-r}(W_r(w)) dr (\langle W_s(\dot{k}_s v), //_s dB_s \rangle + dV_{T-s}(W_s k_s v) ds) \right] \\
= & \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \left(\int_s^T \langle W_r(\dot{k}_r v), //_r dB_r \rangle + dV_{T-r}(W_r k_r v) dr \right) dV_{T-s}(W_s(w)) ds \right]
\end{aligned}$$

which cancels the final three terms in the previous equation, by the strong Markov property, Theorem 2.2 and the assumptions on k . \square

For the case $Z = 0$ and $V = 0$, Theorem 2.7 reduces to [1, Theorem 2.1].

Remark 2.8. We have assumed that V is bounded below and smooth. However, so long as V is bounded below and continuous with $V_t \in C^1$ for each $t \in [0, T]$ and $P^V f \in C^{1,3}([\epsilon, T] \times M)$ then the results of Subsection 2.1 evidently remain valid. Similarly, the results of Subsection 2.2 evidently remain valid if V is bounded below, C^1 with $V_t \in C^2$ for each $t \in [0, T]$ and $P^V f \in C^{1,4}([\epsilon, T] \times M)$. Similarly, the results of Subsection 2.3 evidently remain valid if V is bounded below and continuous with $V_t \in C^2$ for each $t \in [0, T]$ and $P^V f \in C^{1,4}([\epsilon, T] \times M)$.

3 Stationary Solutions

Now suppose $\phi \in C^2(D) \cap C(\overline{D})$ solves the eigenvalue equation

$$(L - V)\phi = -E\phi$$

on the regular domain D , for some $E \in \mathbb{R}$ and a function $V \in C^2$ which does not depend on time and which is bounded below. Denoting by τ the first exit time from D of the diffusion x_t with generator L and assuming $x_0 \in D$, one has, in analogy to the Feynman-Kac formula (3), the formula

$$\phi(x_0) = \mathbb{E} [\mathbb{V}_\tau \phi(x_\tau) e^{E\tau}].$$

Furthermore, the methods of the previous section can easily be adapted to find formulae for the derivatives of ϕ . In particular, one simply sets $f_t = \phi$, replaces V_{T-t} with $V - E$ and the calculations carry over almost verbatim (although there is no application of the strong Markov property; in this case the local martingale property is enough). In particular, for the derivative $d\phi$, supposing k is a bounded adapted process with paths in the Cameron-Martin space $L^{1,2}([0, \infty), \text{Aut}(T_{x_0}M))$ with $k_0 = 1$, $k_t = 0$ for $t \geq \tau$ and $\int_0^\tau |\dot{k}_s|^2 ds \in L^1$, one obtains

$$(d\phi)(v) = -\mathbb{E} \left[\mathbb{V}_\tau \phi(x_\tau) e^{E\tau} \int_0^\tau \langle W_s(\dot{k}_s v), //_s dB_s \rangle + dV(W_s(k_s v)) ds \right]$$

for each $v \in T_{x_0}M$. When $V = 0$ and $E = 0$ this formulae reduces to the one given in [17]. Similarly, denoting by D_1 a regular domain with $x_0 \in D_1$ and $\overline{D_1} \subset D$ and by σ the first exit time of x_t from D_1 , supposing k, l are bounded adapted processes with paths in the Cameron-Martin space $L^{1,2}([0, \infty); \text{Aut}(T_{x_0}M))$ such that $k_s = 0$ for $s \geq \sigma$, $k_0 = 1$, $l_s = 1$ for $s \leq \sigma$, $l_s = 0$ for $s \geq \sigma$, $\int_0^\sigma |\dot{k}_s|^2 ds \in L^1$ and $\int_\sigma^\tau |\dot{l}_s|^2 ds \in L^1$, for the Hessian of ϕ one obtains

$$\begin{aligned} & (\nabla d\phi)(v, w) \\ &= -\mathbb{E} \left[\mathbb{V}_\sigma \phi(x_\sigma) e^{E\sigma} \int_0^\sigma \langle W'_s(\dot{k}_s v, w), //_s dB_s \rangle \right] \\ & \quad - \mathbb{E} \left[\mathbb{V}_\sigma \phi(x_\sigma) e^{E\sigma} \int_0^\sigma ((\nabla dV)(W_s(k_s v), W_s(w)) + (dV)(W'_s(k_s v, w))) ds \right] \\ & \quad + \mathbb{E} \left[\mathbb{V}_\tau \phi(x_\tau) e^{E\tau} \left(\int_0^\tau \langle W_s(\dot{l}_s w), //_s dB_s \rangle + dV(W_s(l_s w)) ds \right) \right. \\ & \quad \quad \left. \cdot \left(\int_0^\sigma \langle W_s(\dot{k}_s v), //_s dB_s \rangle + dV(W_s(k_s v)) ds \right) \right] \end{aligned}$$

for all $v, w \in T_{x_0}M$.

4 Local and Global Estimates

4.1 Gradient

Theorem 4.1. Suppose D_0, D are regular domains with $x_0 \in \overline{D_0} \subset D$, V bounded below and $T > 0$. Set

$$\begin{aligned}\kappa_D &:= \inf\{\text{Ric}_Z(v, v) : v \in T_y M, y \in D, |v| = 1\}; \\ v_D &:= \sup\{|(dV_t)_y(v)| : v \in T_y M, y \in D, |v| = 1, t \in [0, T]\}.\end{aligned}$$

Then there exists a positive constant $C \equiv C(n, T, \inf V, \kappa_D, v_D)$ such that

$$|dP_t^V f_{x_0}| \leq \frac{C}{\sqrt{t}} |f|_\infty \quad (12)$$

for all $0 < t \leq T$, $x_0 \in D_0$ and $f \in \mathcal{B}_b$.

Proof. According to [1], the process k_t appearing in Theorem 2.2 can be chosen so that $|k_s| \leq c(T)$ for all $s \in [0, T]$, almost surely, with

$$\mathbb{E} \left[\int_0^T |\dot{k}_s|^2 ds \right]^{\frac{1}{2}} \leq \frac{\tilde{C}}{\sqrt{1 - e^{-\tilde{C}^2 T}}}$$

for a positive constant \tilde{C} which depend continuously on κ, n and $d(\partial D_0, \partial D)$. The details of this can be found in [18]. By Theorem 2.2 and the Cauchy-Schwarz inequality we have

$$|dP_T^V f| \leq |f|_\infty e^{(-\inf V - \frac{1}{2}(\kappa_D \wedge 0))T} \left(\mathbb{E} \left[\int_0^T |\dot{k}_s|^2 ds \right]^{\frac{1}{2}} + v_D \mathbb{E} \left[\left(\int_0^T |k_s| ds \right)^2 \right]^{\frac{1}{2}} \right)$$

so the estimate (12) follows by substituting the bounds on k and \dot{k} . \square

Corollary 4.2. Suppose Ric_Z is bounded below with $|dV|$ bounded and V bounded below. Then for all $T > 0$ there exists a positive constant $C \equiv C(n, T)$ such that

$$|dP_t^V f_x| \leq \frac{C}{\sqrt{t}} |f|_\infty$$

for all $0 < t \leq T$, $x \in M$ and $f \in \mathcal{B}_b$.

Proof. As explained in the proof of Theorem 4.1, the dependence on D_0 of the constant appearing there is via the quantity $d(\partial D_0, \partial D)$. If M is compact then the injectivity radius $\text{inj}(M)$ is positive and we can choose $D_0 = B_{\text{inj}(M)/4}(x_0)$ and $D = B_{\text{inj}(M)/2}(x_0)$, in which case $d(\partial D_0, \partial D) = \text{inj}(M)/4$. Conversely, if M is non-compact then for each $x_0 \in M$ there exist D_0, D with $x_0 \in \overline{D_0} \subset D$ and $d(\partial D_0, \partial D) = 1$. Consequently, the result follows from Theorem 4.1. \square

4.2 Generator

Theorem 4.3. Suppose D_0, D_1, D_2 are regular domains with $x_0 \in \overline{D_0} \subset D_1$, $\overline{D_1} \subset D_2$, V bounded below and $T > 0$. Set

$$\begin{aligned}\kappa_{D_2} &:= \sup\{|\text{Ric}_Z(v, v)| : v \in T_y M, y \in D_2, |v| = 1\}; \\ v_{D_2} &:= \sup\{|(dV_t)_y(v)| : v \in T_y M, y \in D_2, |v| = 1, t \in [0, T]\}; \\ z_{D_1} &:= \sup\{|Z|_y : y \in D_1\}.\end{aligned}$$

Then there exists a positive constant $C \equiv C(n, T, \inf V, \kappa_{D_2}, v_{D_2}, z_{D_1})$ such that

$$|LP_t^V f_{x_0}| \leq \frac{C}{t} |f|_\infty$$

for all $0 < t \leq T$, $x_0 \in D_0$ and $f \in \mathcal{B}_b$.

Proof. According to [1], the processes k_t and l_t appearing in Theorem 2.5 can be chosen so that

$$\begin{aligned} |k_s| &\leq c_1(n, \kappa_{D_1}, T, d(\partial D_0, \partial D_1)), \\ |l_s| &\leq c_2(n, \kappa_{D_2}, T, d(\partial D_0, \partial D_2)) \end{aligned}$$

for all $s \in [0, T]$, almost surely, with

$$\mathbb{E} \left[\int_0^T |\dot{k}_s|^2 ds \right]^{\frac{1}{2}} \leq \frac{\tilde{C}_1}{\sqrt{1 - e^{-\tilde{C}_1^2 T}}}, \quad \mathbb{E} \left[\int_0^T |\dot{l}_s|^2 ds \right]^{\frac{1}{2}} \leq \frac{\tilde{C}_2}{\sqrt{1 - e^{-\tilde{C}_2^2 T}}}$$

for positive constants \tilde{C}_1 and \tilde{C}_2 which depend continuously on κ , n and on $d(\partial D_0, \partial D_1)$ and $d(\partial D_0, \partial D_2)$, respectively. By Theorem 2.5 and the Cauchy-Schwarz inequality we have

$$\begin{aligned} &|L(P_T^V f)(x_0)| \\ &\leq e^{-\inf V} |f|_\infty z_{D_1} \mathbb{E} \left[\int_0^T |\dot{k}_s|^2 ds \right]^{\frac{1}{2}} \\ &\quad + \frac{1}{2} |f|_\infty e^{T(\kappa_{D_2} - \inf V)} \mathbb{E} \left[\int_0^T |\dot{k}_s|^2 ds \right]^{\frac{1}{2}} \left(\mathbb{E} \left[\int_0^T |\dot{l}_s|^2 ds \right]^{\frac{1}{2}} + v_{D_2} \mathbb{E} \left[\int_0^T |\dot{l}_s|^2 ds \right]^{\frac{1}{2}} \right) \end{aligned}$$

so the result follows by substituting the bounds on k, \dot{k}, l and \dot{l} . \square

Corollary 4.4. Suppose $|\text{Ric}_Z|$, $|dV|$, $|Z|$, are bounded with V bounded below. Then there exists a positive constant $C \equiv C(n, T)$ such that

$$|LP_t^V f_x| \leq \frac{C}{t} |f|_\infty$$

for all $0 < t \leq T$, $x \in M$ and $f \in \mathcal{B}_b$.

Proof. The result follows from Theorem 4.3, since as in Corollary 4.2 any dependence of the constant on D_0, D_1 and D_2 can be eliminated. \square

4.3 Hessian

Theorem 4.5. Suppose D_0, D_1, D_2 are regular domains with $x_0 \in \overline{D_0} \subset D_1$, $\overline{D_1} \subset D_2$, V bounded below and $T > 0$. Set

$$\begin{aligned} \kappa_{D_2} &:= \sup\{|\text{Ric}_Z(v, v)| : v \in T_y M, y \in D_2, |v| = 1\}; \\ v_{D_2} &:= \sup\{|(dV_t)_y(v)| : v \in T_y M, y \in D_2, |v| = 1, t \in [0, T]\}; \\ v'_{D_1} &:= \sup\{|(\nabla dV_t)_y(v, v)| : v \in T_y M, y \in D_1, |v| = 1, t \in [0, T]\}; \\ \rho_{D_1} &:= \sup\{|R(w, v)v| : v, w \in T_y M, y \in D_1, |v| = |w| = 1\}; \\ \rho'_{D_1} &:= \sup\{|(\nabla \text{Ric}_Z^\sharp + d^* R)(v, v)| : v \in T_y M, y \in D_1, |v| = 1\}. \end{aligned}$$

Then there exists a positive constant $C \equiv C(n, T, \inf V, \kappa_{D_2}, v_{D_2}, v'_{D_1}, \rho_{D_1}, \rho'_{D_1})$ such that

$$|\nabla dP_t^V f_{x_0}| \leq \frac{C}{t} |f|_\infty$$

for all $0 < t \leq T$, $x_0 \in D_0$ and $f \in \mathcal{B}_b$.

Proof. Recalling the defining equation for $W'_s(v, w)$, choose the processes k_t and l_t as in the proof of Theorem 4.3 and so that additionally k satisfies

$$\begin{aligned} \mathbb{E} \left[\left(\int_0^T \langle \dot{k}_s W_s \int_0^s W_r^{-1} R(//_r dB_r, W_r) W_r, //_s dB_s \rangle \right)^2 \right]^{\frac{1}{2}} &\leq \frac{\tilde{C}_3 e^{\kappa_{D_1} T}}{\sqrt{1 - e^{-\tilde{C}_3^2 T}}}, \\ \mathbb{E} \left[\left(\int_0^T \langle \dot{k}_s W_s \int_0^s W_r^{-1} (\nabla \text{Ric}_Z^\sharp + d^* R)(W_r, W_r) dr, //_s dB_s \rangle \right)^2 \right]^{\frac{1}{2}} &\leq \frac{\tilde{C}_4 e^{\kappa_{D_1} T}}{\sqrt{1 - e^{-\tilde{C}_4^2 T}}} \end{aligned}$$

for positive constants \tilde{C}_3 and \tilde{C}_4 which depend continuously on κ_{D_1} , ρ_{D_1} , ρ'_{D_1} , n and on $d(\partial D_0, \partial D_1)$. Such k can always be chosen; the details of this are found in [14, Section 4.2], with appropriate bounds for the radial part of the diffusion being given as in the proof of [20, Corollary 2.1.2]. By Theorem 2.7 and the Cauchy-Schwarz inequality we have

$$\begin{aligned} &|\nabla dP_T^V f| \\ &\leq |f|_\infty e^{T(\kappa_{D_2} - \inf V)} \left(\frac{\tilde{C}_3}{\sqrt{1 - e^{-\tilde{C}_3^2 T}}} + \frac{1}{2} \frac{\tilde{C}_4}{\sqrt{1 - e^{-\tilde{C}_4^2 T}}} \right) \\ &\quad + |f|_\infty e^{T(\kappa_{D_2} - \inf V)} \left(v'_{D_1} \mathbb{E} \left[\left(\int_0^T |k_s| ds \right)^2 \right]^{\frac{1}{2}} + v_{D_2} c_1^2(\rho_{D_1} \vee \frac{1}{2} \rho'_{D_1}) \frac{T^2}{\sqrt{2}} \right) \\ &\quad + |f|_\infty e^{T(\kappa_{D_2} - \inf V)} \left(\mathbb{E} \left[\int_0^T |\dot{l}_s|^2 ds \right]^{\frac{1}{2}} + v_{D_2} \mathbb{E} \left[\left(\int_0^T |l_s| ds \right)^2 \right]^{\frac{1}{2}} \right) \\ &\quad \cdot \left(\mathbb{E} \left[\int_0^T |\dot{k}_s|^2 ds \right]^{\frac{1}{2}} + v_{D_2} \mathbb{E} \left[\int_0^T |k_s|^2 ds \right]^{\frac{1}{2}} \right) \end{aligned}$$

so the result follows by substituting the bounds on k, \dot{k}, l and \dot{l} . \square

Corollary 4.6. Suppose $|\text{Ric}_Z|$, $|dV|$, $|\nabla dV|$, $|\nabla \text{Ric}_Z^\sharp + d^* R|$ and $|R|$ are bounded with V bounded below. Then there exists a positive constant $C \equiv C(n, T)$ such that

$$|\nabla dP_t^V f_x| \leq \frac{C}{t} |f|_\infty$$

for all $0 < t \leq T$, $x \in M$ and $f \in \mathcal{B}_b$.

Proof. The result follows from Theorem 4.5, since as in Corollaries 4.2 and 4.4 any dependence of the constant on D_0 , D_1 and D_2 can be eliminated. \square

5 Non-local Formulae

If Ric_Z is bounded below then, by [20, Corollary 2.1.2], the diffusion x_t is non-explosive, which is to say $\zeta(x_0) = \infty$, almost surely. While the formulae in this section require non-explosion and global bounds on the various curvature operators, they are expressed in terms of explicit and deterministic processes k and l .

Theorem 5.1. Suppose $x_0 \in M$ with $v \in T_{x_0} M$, $f \in \mathcal{B}_b$, V bounded below and $T > 0$. Set

$$k_s = \frac{T - s}{T}.$$

Suppose Ric_Z is bounded below with $|dV|$ bounded and V bounded below. Then

$$(dP_T^V f)(v) = -\mathbb{E} \left[\mathbb{V}_T f(x_T) \int_0^T \langle W_s(\dot{k}_s v), //_s dB_s \rangle + dV_{T-s}(W_s(k_s v)) ds \right].$$

Proof. It follows from Corollary 4.2 that $|dP_t^V|$ is bounded on $[\epsilon, T] \times M$. Therefore, using

$$k_s^\epsilon = \frac{T - \epsilon - s}{T - \epsilon} \vee 0$$

the local martingale (4) is a true martingale. Taking expectations and eliminating ϵ with dominated convergence yields the above formula. \square

Theorem 5.1 is precisely [5, Theorem 5.2], which was also obtained in [11] by a slightly different method.

Theorem 5.2. Suppose $x_0 \in M$, $f \in \mathcal{B}_b$, V bounded below and $T > 0$. Set

$$k_s = \frac{T - 2s}{T} \vee 0, \quad l_s = 1 \wedge \frac{2(T - s)}{T}.$$

Suppose $|\text{Ric}_Z|$, $|dV|$ and $|Z|$ are bounded with V bounded below. Then

$$\begin{aligned} & L(P_T^V f)(x_0) \\ &= \mathbb{E} \left[\mathbb{V}_T f(x_T) \int_0^T \langle \dot{k}_s Z, //_s dB_s \rangle \right] \\ &+ \frac{1}{2} \mathbb{E} \left[\mathbb{V}_T f(x_T) \left(\int_0^T \langle W_s \dot{l}_s, //_s dB_s \rangle + dV_{T-s}(W_s l_s) ds \right) \int_0^T \dot{k}_s W_s^{-1} //_s dB_s \right]. \end{aligned}$$

Proof. It follows from Corollary 4.4 that $|LP_t^V|$ is bounded on $[\epsilon, T] \times M$. Therefore, using k_s and

$$l_s^\epsilon = \left(1 \wedge \frac{T - \epsilon - s}{\frac{T}{2} - \epsilon} \right) \vee 0$$

the local martingale appearing in Lemma 2.3 is a true martingale. Taking expectations, using Lemma 2.4 as in the proof of Theorem 2.5 and eliminating ϵ with dominated convergence yields the above formula. \square

Theorem 5.3. Suppose $x_0 \in M$ with $v, w \in T_{x_0} M$, $f \in \mathcal{B}_b$, V bounded below and $T > 0$. Define k_s and l_s as in Theorem 5.2. Suppose $|\text{Ric}_Z|$, $|dV|$, $|\nabla dV|$, $|\nabla \text{Ric}_Z^\sharp + d^* R|$ and $|R|$ are bounded with V bounded below. Then

$$\begin{aligned} & (\nabla dP_T^V f)(v, w) \\ &= -\mathbb{E} \left[\mathbb{V}_T f(x_T) \int_0^T \langle W'_s(\dot{k}_s v, w), //_s dB_s \rangle \right] \\ &- \mathbb{E} \left[\mathbb{V}_T f(x_T) \int_0^T ((\nabla dV_{T-s})(W_s(k_s v), W_s(w)) + (dV_{T-s})(W'_s(k_s v, w))) ds \right] \\ &+ \mathbb{E} \left[\mathbb{V}_T f(x_T) \left(\int_0^T \langle W_s(\dot{l}_s w), //_s dB_s \rangle + dV_{T-s}(W_s(l_s w)) ds \right) \right. \\ &\quad \left. \cdot \left(\int_0^T \langle W_s(\dot{k}_s v), //_s dB_s \rangle + dV_{T-s}(W_s(k_s v)) ds \right) \right]. \end{aligned}$$

Proof. It follows from Corollary 4.6 that $|dP_t^V|$ and $|\nabla dP_t^V|$ are bounded on $[\epsilon, T] \times M$. Therefore, using l_s^ϵ defined as in the proof of Theorem 5.2, the local martingale appearing in Lemma 2.6 is a true martingale. Taking expectations, proceeding as in the proof of Theorem 2.7 and eliminating ϵ with dominated convergence yields the above formula. \square

For the case $V = 0$, Theorem 5.3 gives the filtered version of the second part of [5, Theorem 3.1], which was proved by differentiating under the expectation for $f \in BC^2$ and which, as observed in [14], contains a slight error, permuting the vectors v and w .

Remark 5.4. *It is evident that our formulae require either $V \in C^1$ or $V \in C^2$ (see Remark 2.8). More generally it is desirable to consider possibly very singular potentials (see for example [7]), such as those which appear in many quantum mechanical problems. It was pointed out to the authors of [5] by G. Da Prato, and to the author of this article by X.-M. Li, that under certain conditions the case of non-smooth V be dealt with using the variation of constants formula. If P_T denotes the minimal semigroup associated to the operator L then the variation of constants formula implies*

$$P_T^V f = P_T f - \int_0^T P_{T-s}(V_s P_s^V f) ds.$$

So long as P_T^V is sufficiently regular, formulae and estimates for $P_T^V f$ and its gradient can be obtained from formulae and estimates for $P_T f$ and its gradient, simply by differentiating the above formula and substituting. For the second derivatives one must take care in passing these derivatives through the integral. For the case in which the potential is a bounded Hölder continuous function V which does not depend on time, this can be achieved at each point $x_0 \in M$ by shifting V to $V(x_0) = 0$. The details of this for the Hessian, are given in [10], where the approach taken is based on that of [5].

6 Kernel Estimates

Now suppose $Z = \nabla h$, for some $h \in C^2$, and consider the m -dimensional Bakry-Emery curvature tensor

$$\text{Ric}_{m,n} := \text{Ric}^\sharp + \nabla dh - \frac{\nabla h \otimes \nabla h}{m - n}$$

where $m \geq n$ is a constant (see [13]). Denoting by $p_t^h(x, y)$ the density of the diffusion with generator L , with respect to the weighted Riemannian measure $e^h dy$, it follows, as explained in the proof of [9, Theorem 1.4], that if $\text{Ric}_{m,n} \geq -\kappa$ for some $\kappa \geq 0$ then there exists a positive constant $C \equiv C(\kappa, m, T)$ such that

$$\log \left(\frac{p_{\frac{t}{2}}^h(x, z)}{p_t^h(x, y)} \right) \leq C \left(1 + \frac{d^2(x, y)}{t} \right)$$

for all $x, y, z \in M$ and $t \in (0, T]$. Assuming V is bounded, it follows that the same inequality holds for the integral kernel $p_t^{h,V}(x, y)$ of the semigroup $P_t^V f$, since

$$p_t^{h,V}(x, y) = p_t^h(x, y) \mathbb{E}[\mathbb{V}_t | x_0 = x, x_t = y]$$

by the Feynman-Kac formula. It is thus a simple matter to derive from Theorems 5.1, 5.2 and 5.3 estimates on the logarithmic derivatives of $p_t^{h,V}(x, y)$ by a standard argument based on Jensen's inequality (see [15, Lemma 6.45]). In particular, the assumptions of

Theorem 5.1 with $Z = \nabla h$ plus boundedness of V and a lower bound on $\text{Ric}_{m,n}$ imply the existence of a constant $C_1(T)$ such that

$$|d \log p_t^{h,V}(\cdot, y)_x|^2 \leq C_1(T) \left(\frac{1}{t} + \frac{d^2(x, y)}{t^2} \right)$$

for all $x, y \in M$ and $t \in (0, T]$. The details of this (for the case $h = 0$) can be found in [11]. Similarly, the assumptions of Theorem 5.2 with $Z = \nabla h$ plus boundedness of V and a lower bound on $\text{Ric}_{m,n}$ imply for the Witten Laplacian $\Delta_h := \frac{1}{2}\Delta + \nabla h$ the existence of a constant $C_2(T)$ such that

$$|\Delta_h \log p_t^{h,V}(\cdot, y)(x)| \leq C_2(T) \left(\frac{1}{t} + \frac{d^2(x, y)}{t^2} \right)$$

for all $x, y \in M$ and $t \in (0, T]$. Finally, the assumptions of Theorem 5.3 with $Z = \nabla h$ plus boundedness of V and a lower bound on $\text{Ric}_{m,n}$ imply the existence of a constant $C_3(T)$ such that

$$|\nabla d \log p_t^{h,V}(\cdot, y)_x| \leq C_3(T) \left(\frac{1}{t} + \frac{d^2(x, y)}{t^2} \right)$$

for all $x, y \in M$ and $t \in (0, T]$.

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